

# A Renormalization Group Method for Quasi One-dimensional Quantum Hamiltonians

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A density-matrix renormalization group (DMRG) method for highly anisotropic two-dimensional systems is presented. The method consists in applying the usual DMRG in two steps. In the first step, a pure one dimensional calculation along the longitudinal direction is made in order to generate a low energy Hamiltonian. In the second step, the anisotropic 2D lattice is obtained by coupling in the transverse direction the 1D Hamiltonians. The method is applied to the anisotropic quantum spin half Heisenberg model on a square lattice.

The density-matrix renormalization group method introduced by White [1] a decade ago has proven a remarkable efficiency in the computation of the ground-state [2, 3, 4], thermodynamic [5, 6] and dynamic [7, 8] properties of one-dimensional interacting electron models as well as electron-phonon systems [9, 10]. An extension of the method to two dimensional systems is currently the object of some efforts [11]. But an efficient 2D algorithm is still lacking.

An interesting situation which has been so far overlooked is the possible application of the DMRG technique to strongly anisotropic 2D systems. In such systems, the interaction Hamiltonian can be written as the sum of two terms:  $H = H_{\parallel} + gH_{\perp}$ ; where  $H_{\parallel}$  is the sum over one-dimensional (1D) Hamiltonians (longitudinal direction) and  $H_{\perp}$  is the interaction between these 1D systems (transverse direction).  $H_{\parallel}$  and  $H_{\perp}$  are of the same magnitude and  $g \ll 1$ . This type of situation arises in various physical systems including quasi 1D organic and inorganic materials, weakly coupled ladder systems, carbon nanotube ropes, quasi 1D antiferromagnets, quasi 1D spin-Peierls systems, etc. It is the purpose of this letter to show that a DMRG algorithm can be implemented for the study of such anisotropic models.

The standard approach to anisotropic Hamiltonians such as  $H$  is to first diagonalize  $H_{\parallel}$  and then use its eigenstates to compute the corrections introduced by  $H_{\perp}$ . We present below an algorithm which follows this spirit. This method consists in applying a two-step DMRG method to Hamiltonians having the form of  $H$ . The standard DMRG is first used along the longitudinal direction until the scale of  $gH_{\perp}$  is reached. Then a transformation is made in order to keep only a small number (a few tens) of low lying states of  $H_{\parallel}$ . These states are then used as a starting point for a second DMRG calculation along the transverse direction. The validity of this procedure is discussed. As in the thermodynamic algorithm [5] which was introduced by the authors, the accuracy depends on not only the number of states  $m$  kept by blocks, but also

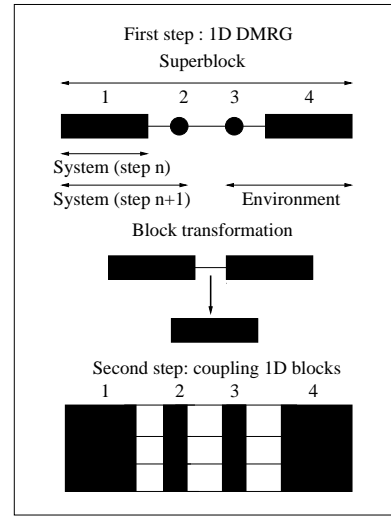


FIG. 1: Sketch of the two-step density-matrix renormalization group algorithm

on the number of the target states  $M$ .

The two-step DMRG is illustrated in Fig. 1. The first step of the quasi 1D algorithm is the usual 1D DMRG method. For the sake of completeness, we briefly recall the main steps of the algorithm. For more details, we refer the reader to the more extensive presentations in ref[4]. An iteration of the DMRG algorithm with the infinite system method proceeds as follows: (a) the Hamiltonian for the superblock 1+2+3+4 (where the blocks 1 and 4 come from previous iterations and 2 and 3 are new added ones. Blocks 2 and 3 are usually single site blocks) is diagonalized in order to obtain the few  $M$  lowest lying wave functions  $|\Psi_k(1, 2, 3, 4)\rangle$ ,  $k = 1, M$ . (b) the reduced density matrix of blocks 1+2 is constructed. This reduced density matrix is  $\rho = \sum_k \omega_k \rho_k$ , where  $\rho_k$  and  $\omega_k$  are respectively the reduced density matrix of the  $k^{th}$  state and its weight.  $\rho_k$  is related to the superblock wave function  $\Psi_k(1, 2, 3, 4)$  through the relation,  $\rho_k(1, 2; 1', 2') = \sum_{3,4} |\Psi_k(1, 2, 3, 4)\rangle \langle \Psi_k^*(1', 2', 3, 4)|$ .

$\rho$  is diagonalized and the  $m$  eigenstates with the highest eigenvalues  $\lambda_\alpha$  are kept. Since  $\sum_\alpha \lambda_\alpha = 1$ , because  $\rho$  is a density matrix, the error made by truncating this sum to  $m$  states is  $p_m = 1 - \sum_{\alpha=1,m} \lambda_\alpha$ . (c) These states form a new reduced basis in which all the operators have to be expanded and the block 1+2 is renamed as block 1. New block 2 and 3 are added to form a new superblock. This procedure is repeated until one reaches the desired lattice size. This means typically, once the energy separation between the eigenstates of the 1D system are of the same magnitude as  $g$ .

Once the size  $L + 2$  of the superblock is large enough, *i.e.* when the difference between the first excited state and the ground state is such that  $|E_0 - E_1| \approx g$ , we perform a block transformation, of the type of the old RG method [12, 13], on blocks 1 and 4. The two  $L/2$ -lattices with  $m$  states are coupled, then renormalized to a  $L$ -lattice with  $m$  states. These  $m$  states are the ground state and the low-lying excited states of the  $L$ -lattice. They can now be coupled through  $g$ . One can note that the boundary condition problem in the block RG method raised by White and Noack [14] does not exist here, this is because the block transformation is only applied once. A 2D lattice is then generated by using the 1D density-matrix renormalization group algorithm with chains as units instead of sites.

This new block 1 will serve, in the second DMRG step, as a building unit for a new series of iteration that are similar to those performed in step 1. This block is labelled block 2 in the second step since it plays the role played by a single site in step 1. This two-step method can be justified as follows: in the study of the ground state properties of a quasi 1D system, since  $g \ll 1$ ,  $gH_\perp$  may be neglected in the early steps of the renormalization process. The reason is that finite size effects act as temperature. When the size is small, the excitation energies are far greater than the transverse coupling,  $g \ll |E_0 - E_n|$ , therefore  $g$  is irrelevant.

We now illustrate the two-step DMRG method in the case of weakly coupled spin-half Heisenberg chains on a square lattice. The Hamiltonian reads,

$$H_{spins} = \sum_{i,l} \mathbf{S}_{i,l} \mathbf{S}_{i+1,l} + J_\perp \sum_{i,l} \mathbf{S}_{i,l} \mathbf{S}_{i,l+1} \quad (1)$$

where the  $\mathbf{S}_{i,l}$  are the usual spin-half operators. Following the prescriptions above, we start by applying the 1D DMRG on the single chain Hamiltonian  $H_{\parallel,l} = \sum_i \mathbf{S}_{i,l} \mathbf{S}_{i+1,l}$ . It was shown by White [1] that a relatively small number of  $m$  states kept in block 1 can lead to an astonishingly high accuracy for the ground-state energy and spin correlation functions. An accuracy ranging from  $10^{-6}$  to better than  $10^{-10}$  for the ground state energy of a  $L = 28$  sites chain was obtained by keeping only  $m = 16$  to  $m = 64$  states with modest computational power.

$m$	1D	Ladder 1	Ladder 2	2D
16	-13.98792	-13.62493	-14.00113	-14.07066
24	-13.99650	-13.69023	-14.01248	-14.08803
32	-13.99724	-13.70638	-14.01526	-14.09810
40	-13.99729	-13.71446	-14.01749	-14.10489

TABLE I: Ground state energies per chain of single chain (1D) with  $L = 32$ , of a two-leg ladder  $2 \times L$  obtained with the usual DMRG (Ladder 1), of the same ladder obtained with the two-step method (Ladder 2), of a  $32 \times 32$  system (2D).

A set of these highly accurate low energy eigenstates  $|\phi_{n_l}\rangle$  and eigenvalues  $\epsilon_{n_l}$  of  $H_{\parallel,l}$  is first obtained by the 1D DMRG. The eigensets of the disconnected chain Hamiltonian  $H_{\parallel} = \sum_l H_{\parallel,l}$  are given by the relations:

$$\Phi_{[n]} = \prod_l |\phi_{n_l}\rangle, \quad E_{[n]} = \sum_l \epsilon_{n_l} \quad (2)$$

$[n] = (n_1, n_2, \dots, n_L)$ ,  $n_l$  corresponds to an eigenset on the chain  $l$ . The eigenset  $\Phi_{[n]}$ ,  $E_{[n]}$  diagonalizes  $H_{\parallel}$ :

$$\langle \Phi_{[n]} | H_{\parallel} | \Phi_{[m]} \rangle = E_{[n]} \delta_{[n],[m]}. \quad (3)$$

The matrix elements of  $H_\perp$  in the basis formed by the  $\Phi_{[n]}$  are:

$$\langle \Phi_{[n]} | H_\perp | \Phi_{[m]} \rangle = \sum_l \langle \Phi_{[n]} | \sum_i \mathbf{S}_{i,l} \mathbf{S}_{i,l+1} | \Phi_{[m]} \rangle. \quad (4)$$

This last equation 4 can readily be transformed to:

$$\langle \Phi_{[n]} | H_\perp | \Phi_{[m]} \rangle = \sum_{il} \tilde{\mathbf{S}}_{i,l}^{n_l, m_l} \tilde{\mathbf{S}}_{i,l+1}^{n_{l+1}, m_{l+1}}. \quad (5)$$

where  $\tilde{\mathbf{S}}_{i,l}^{n_l, m_l} = \langle \phi_{n_l} | \mathbf{S}_{i,l} | \phi_{m_l} \rangle$ . The renormalized Hamiltonian  $\tilde{H}$  in the basis of the  $\Phi_{[n]}$  is thus:

$$\tilde{H} \approx \sum_{[n]} E_{[n]} |\Phi_{[n]} \rangle \langle \Phi_{[n]}| + J_\perp \sum_{il} \tilde{\mathbf{S}}_{i,l} \tilde{\mathbf{S}}_{i,l+1}. \quad (6)$$

$\tilde{H}$  is studied by the usual 1D DMRG algorithm. It is however to be noted that the computational requirement for  $\tilde{H}$  are greater than in the study of a simple spin chain performed in the first step. The renormalized spin operators  $\tilde{\mathbf{S}}_{i,l}$  are now  $m \times m$  matrices instead of  $2 \times 2$ . The size of the superblock in the second step is  $m'^2 \times m^2$  (it is  $4 \times m^2$  in step 1) if  $m'$  states are kept in the two external blocks. We were nonetheless able to perform the calculations on a workstation for up to  $m = 48$ .

It is instructive to compare the results which are obtained by the proposed method with a known case. A simple situation is the two-leg spin ladder model. We

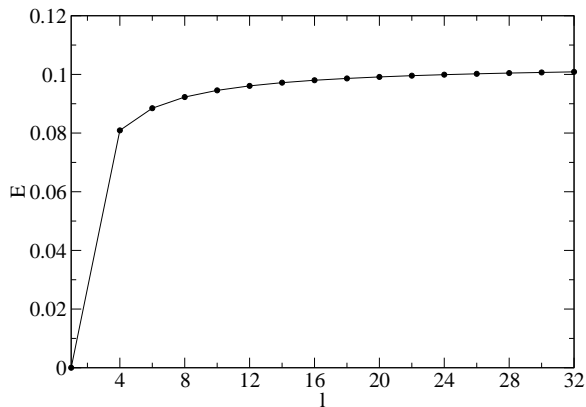


FIG. 2: The binding energy of the  $32 \times l$  system (relative to the isolated 32 site chain) for  $m = 32$  and  $J_{\perp} = 0.1$

$m$	$\Delta(L)$	$\delta E(L)$	$\dim S_z = 0$
16	0.11671	0.58664	12 251
24	0.11780	0.65044	66 850
32	0.11777	0.72977	205 920
40	0.11774	0.78363	477 670

TABLE II: Finite size spin gap  $\Delta(L)$ , band-width of the retained states  $\delta E(L)$  and the dimension of the subspace with  $S_z = 0$  in the two-step method.

have computed the ground state energy of the ladder system in two ways. First, we use the usual DMRG algorithm which have been widely applied for the study of this system during the last decade [16]. Second, we compute the ground-state energy of the two leg ladder by first obtaining the low energy Hamiltonian of a single chain. For this, we targeted  $M = 5$  states corresponding to the lowest states of the spin sectors  $S_z = \pm 2, \pm 1$  and 0. It is necessary to target other spin sectors when building the low energy Hamiltonian because, when forming the tensor product, they may lead to lower energy states than some  $S_z = 0$  states. A criteria for the selection of spin sector to be selected is similar to the one applied in the thermodynamic algorithm. If the lowest state of  $S_z$  is higher than the highest state retained in  $S_z = 0$ , the subspace  $S_z$  is not retained. We then coupled two low energy 1D Hamiltonians with  $J_{\perp}$  to form a ladder. This corresponds to performing the second step of the two-step DMRG with one iteration and two blocks instead of four.

In table I we compare the ground state energies of the ladder obtained by the two methods as well as those of a single chain for  $L = 32$ . The infinite system DMRG method with open boundary conditions was used. The energy per site of the 32 site single chain for  $m = 40$  is  $-0.4374$  which is still far from the exact ground state energy of the infinite chain  $-0.4431$ . This is because chains with open boundary conditions converge very slowly (as

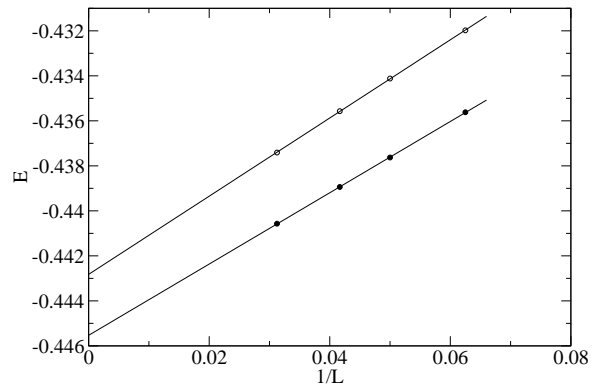


FIG. 3: The ground state energy per site for the 2D lattice for  $J_{\perp} = 0$  (open circles) and  $J_{\perp} = 0.1$  (filled circles) as a function of  $L$  for  $m = 32$ .

$1/L$ ) to the thermodynamic limit. It can be seen that the energy of the two step DMRG are systematically better than those of the simple DMRG. The latter are found to be even higher than those of a single chain. This can be understood by the fact that the DMRG method is less accurate in situations where the ground state is nearly degenerate. This type of situation is, for instance, encountered in the small coupling region of the Kondo lattice [3] where a large number of states must be kept to get reliable results. Another look at this is that when  $J_{\perp}$  is small, the two chains are nearly independent, the  $m$  states are shared between the two chains  $\sqrt{m}$  states for each chain [15].

The ground state energy of the two dimensional system ( $32 \times 32$ ) is shown in the last column of table I and Fig. 2 shows the variation of the ground state energy per chain as a function of the chain number  $l$ , the reference is a single chain with  $L = 32$ . It displays a rapid convergence as  $l$  increases. We kept the same number of states in the two external blocks as in the internal blocks during the second step of the DMRG. Truncation errors are between  $10^{-3}$  and  $10^{-5}$  for  $m = 16$  to 40. One should note, however, that these errors are relative to the truncated Hamiltonian. Hence they do not necessarily represent the accuracy of the method. It is important to verify that the truncated Hamiltonian generated for the single chain is accurate enough, for the ground state and for the low lying state, to be used as a building block for the 2D lattice. This will depend indeed on  $m$  and  $M$ , but also on  $J_{\perp}$  and  $L$ . One can easily see that for a fixed  $L$  and  $J_{\perp} \ll \Delta_{\sigma}(L)$ ,  $\Delta_{\sigma}(L)$  is the finite size spin gap, the interchain matrix elements will be negligible. The system will behave as a collection of free chains even if  $J_{\perp}$  is turned on. Now if  $J_{\perp} \sim \delta E(L)$ ,  $\delta E(L)$  is the width of the retained states, the matrix elements of the states having higher energy which have been truncated out have a non-negligible contribution. We thus expect the two-step DMRG technique to be reliable when  $J_{\perp}$  is within the range  $\Delta_{\sigma}(L) \simeq J_{\perp} \ll \delta E(L)$ . Values of  $\Delta_{\sigma}(L)$

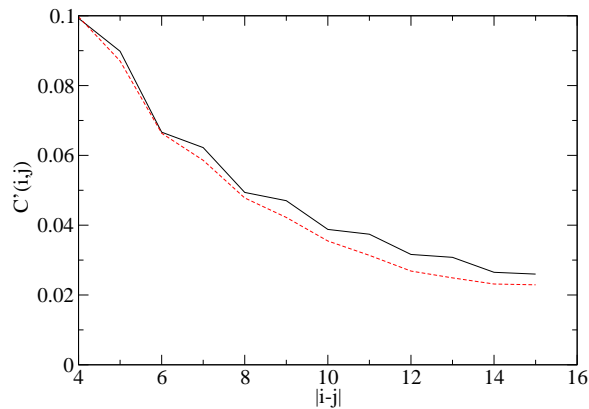


FIG. 4: The averaged ground state correlation function  $C'(i, j) = (-1)^{|i-j|} \langle \mathbf{S}_i \mathbf{S}_j \rangle$  of a single chain (full) and of the  $32 \times 32$  system (dashed) for  $m = 32$  and  $J_{\perp} = 0.1$

and  $\delta E(L)$  are displayed in table II. An estimate of the extrapolated ground state energy per site for the 2D system (Fig. 3) is  $-0.4455$  for  $J_{\perp} = 0.1$  when  $m = 32$  (the same value of  $m$  gives  $-0.4428$  for  $J_{\perp} = 0$ ). This is to be compared to the quantum Monte Carlo (QMC) estimate  $-0.4485$  for the infinite system obtained using clusters with periodic boundary conditions [17].

The possible occurrence of long-range order is studied by observing the behavior of spin correlation functions. This is however complicated by the use of open boundary conditions. It is known that [1, 15] the OBC induce a strong odd-even alternation in the spin correlation functions. This alternation is also observed for the 2D system with  $J_{\perp} = 0.1$ . In order to avoid this alternation, we defined the spin correlation function as the average between these two states. This is done by computing  $\langle \mathbf{S}_1 \mathbf{S}_l \rangle$  in two ways.  $\mathbf{S}_1$  is taken as the origin of a strong link or as the origin on a weak link. This averaging process reduces the even-odd alternation as shown in Fig. 4 for the single chain; the alternation is suppressed in the 2D system. The suppression of the alternation in the 2D system after averaging is probably due to the fact that the valence bond picture is not valid for the 2D system, even with open boundary conditions. The observation of the alternation before averaging is simply reminiscent of the starting point which is a single chain.

We have shown that the DMRG can successfully be applied to highly anisotropic 2D systems. We used the spin-half Heisenberg anisotropic model on a square lattice as a test case. Even in this simple case, the computational power required increases significantly with the

number of block states kept as shown in the last column of Table. II. An analysis of the program reveals that 75 percent of the CPU time is spent during the calculation of the superblock wave function. This step involves mostly matrix-vector products. A significant improvement in speed is thus expected by the use of parallel computers. Furthermore, the initial guess for the superblock wave function was a random vector at each iteration. Another improvement of the program is to use a transformed state from the previous iteration as done in the standard DMRG method [18].

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